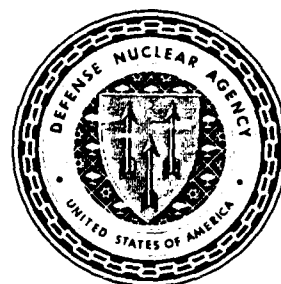




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Alexandria, VA 22310-3398



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## **Radiative Properties of $UO^+$**

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December 1989

Technical Report

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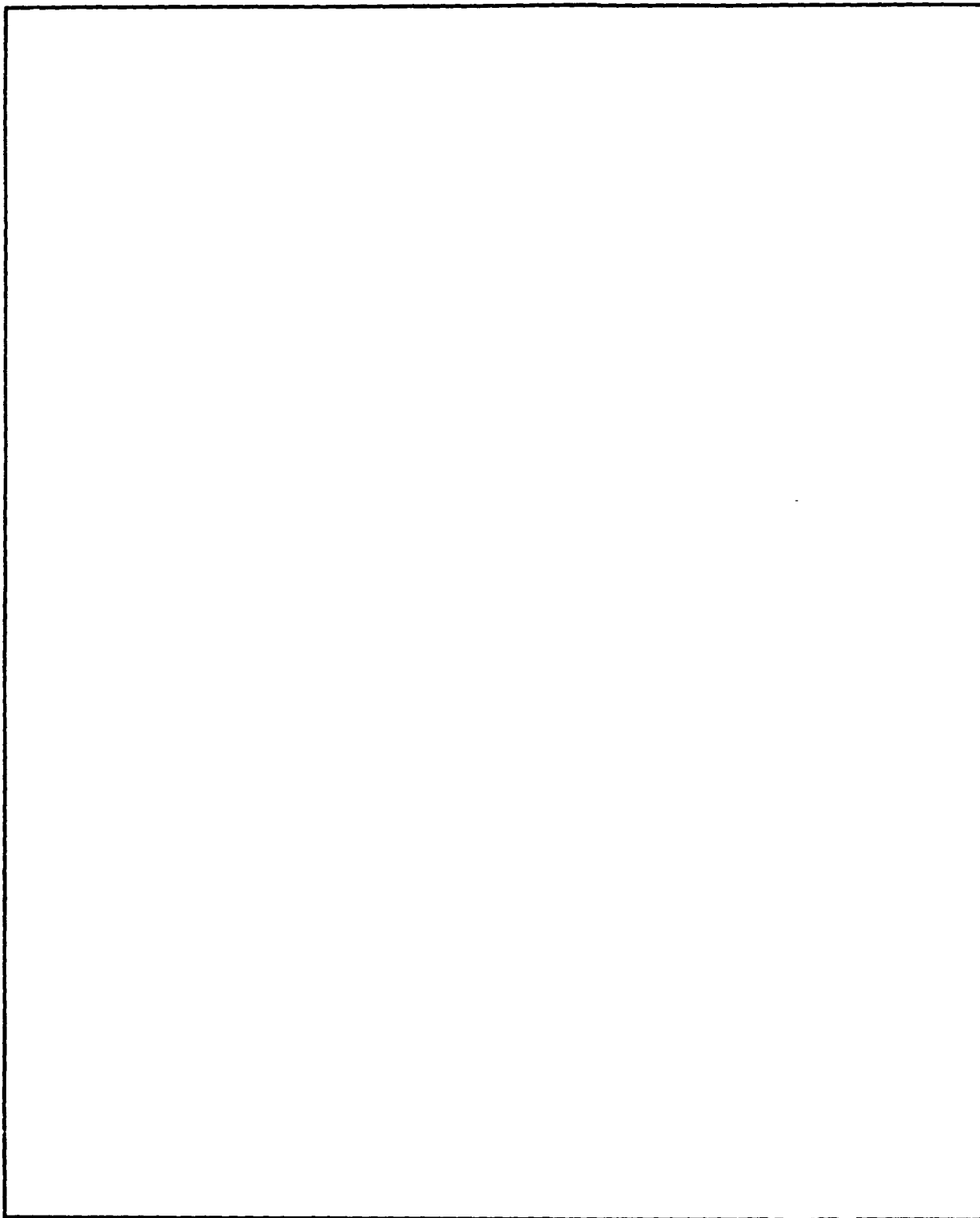
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### Conversion Table

(Conversion factors for U.S. customary to  
metric (SI) units of measurement)

To Convert From	To	Multiply By
angstrom	meters (m)	1.000 000 x E-10
atmosphere (normal)	kilo pascal (kPa)	1.013 25 x E+2
bar	kilo pascal (kPa)	1.000 000 x E+2
barn	meter <sup>2</sup> (m <sup>2</sup> )	1.000 000 x E-28
British thermal unit (thermochemical)	joule (J)	1 054 350 x E+3
cal (thermochemical)/cm <sup>2</sup>	mega joule/m <sup>2</sup> (MJ/m <sup>2</sup> )	4.184 000 x E-2
calorie (thermochemical)	joule (J)	4.184 000
calorie (thermochemical)/g	joule per kilogram (J/kg)	4.184 000 x E+3
curie	giga becquerel (GBq)	3.700 000 x E+1
degree Celsius	degree kelvin (K)	$t_K = t_C + 273.15$
degree (angle)	radian (rad)	1.745 329 x E-2
degree Fahrenheit	degree kelvin (K)	$t_K = (t_F + 459.67)/1.8$
electron volt	joule (J)	1.602 19 x E-19
erg	joule (J)	1.000 000 x E-7
erg/second	watt (W)	1.000 000 x E-7
foot	meter (m)	3.048 000 x E-1
foot-pound-force	joule (J)	1.355 818
gallon (U.S. liquid)	meter <sup>3</sup> (m <sup>3</sup> )	3.785 412 x E-3
inch	meter (m)	2.540 000 x E-2
jerk	joule (J)	1.000 000 x E+9
joule/kilogram (J/kg) (radiation dose absorbed)	gray (Gy)	1.000 000
kilotons	terajoules	4.183
kip (1000 lbf)	newton (N)	4.448 222 x E+3
kip/inch <sup>2</sup> (ksi)	kilo pascal (kPa)	6.894 757 x E+3
ktap	newton-second/m <sup>2</sup> (N-s/m <sup>2</sup> )	1.000 000 x E+2
micron	meter (m)	1.000 000 x E-6

Conversion Table (Concluded)

To Convert From	To	Multiply By
mil	meter (m)	2.540 000 x E-5
mile (international)	meter (m)	1.609 344 x E+3
ounce	kilogram (kg)	2.834 952 x E-2
pound-force (lbf avoirdupois)	newton (N)	4.448 222
pound-force inch	newton-meter (N·m)	1.129 848 x E-1
pound-force/inch	newton/meter (N/m)	1.751 268 x E+2
pound-force/foot <sup>2</sup>	kilo pascal (kPa)	4.788 026 x E-2
pound-force/inch <sup>2</sup> (psi)	kilo pascal (kPa)	6.894 757
pound-mass (lbm avoirdupois)	kilogram (kg)	4.535 924 x E-1
pound-mass-foot <sup>2</sup> (moment of inertia)	kilogram-meter <sup>2</sup> (kg·m <sup>2</sup> )	4.214 011 x E-2
pound-mass/foot <sup>3</sup>	kilogram-meter <sup>3</sup> (kg/m <sup>3</sup> )	1.601 846 x E+1
rad (radiation dose absorbed)	gray (Gy)	1.000 000 x E-2
roentgen	coulomb/kilogram (C/kg)	2.579 760 x E-4
shake	second (s)	1.000 000 x E-8
slug	kilogram (kg)	1.459 390 x E+1
torr (mm Hg, 0°C)	kilo pascal (kPa)	1.333 22 x E-1

## TABLE OF CONTENTS

Section	Page
Conversion Table	iii
List of Tables	vi
1 Radiative Properties of UO <sup>+</sup>	1
2 List of References	17

<b>Accession For</b>	
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## LIST OF TABLES

Table		Page
1	Calculated oscillator strengths $f_{(v',v'')}$ for the $1^4\text{I} - 1^4\text{K}$ transition of $\text{UO}^+$ .	4
2	Calculated oscillator strengths $f_{(v',v'')}$ for the $1^4\text{I} - 3^4\text{H}$ transition of $\text{UO}^+$ .	5
3	Calculated oscillator strengths $f_{(v',v'')}$ for the $1^4\text{I} - 2^4\text{H}$ transition of $\text{UO}^+$ .	6
4	Calculated oscillator strengths $f_{(v',v'')}$ for the $1^4\text{I} - 1^4\text{H}$ transition of $\text{UO}^+$ .	7
5	Calculated oscillator strengths $f_{(v',v'')}$ for the $1^4\text{I} - 2^4\text{I}$ transition of $\text{UO}^+$ .	8
6	Calculated oscillator strengths $f_{(v',v'')}$ for the $1^4\text{I} - 1^6\text{H}$ transition of $\text{UO}^+$ .	9
7	Calculated oscillator strengths $f_{(v',v'')}$ for the $1^4\text{I} - 3^4\text{I}$ transition of $\text{UO}^+$ .	10
8	Calculated oscillator strengths $f_{(v',v'')}$ for the $1^4\text{H} - 2^4\text{I}$ transition of $\text{UO}^+$ .	11
9	Calculated oscillator strengths $f_{(v',v'')}$ for the $1^4\text{H} - 2^4\text{H}$ transition of $\text{UO}^+$ .	12
10	Calculated oscillator strengths $f_{(v',v'')}$ for the $1^4\text{H} - 1^4\text{K}$ transition of $\text{UO}^+$ .	13
11	Calculated oscillator strengths $f_{(v',v'')}$ for the $1^4\text{H} - 1^6\text{H}$ transition of $\text{UO}^+$ .	14
12	Calculated oscillator strengths $f_{(v',v'')}$ for the $1^4\text{H} - 3^4\text{H}$ transition of $\text{UO}^+$ .	15
13	Calculated oscillator strengths $f_{(v',v'')}$ for the $1^4\text{H} - 3^4\text{I}$ transition of $\text{UO}^+$ .	16



## SECTION 1

### RADIATIVE PROPERTIES OF $\text{UO}^+$

An analysis of the electronic structure of  $\text{UO}$  and  $\text{UO}^+$  using a relativistic formulation has been undertaken (References 1 and 2). Preliminary calculations were performed for several states of  $\text{UO}$  and  $\text{UO}^+$  and for the ground and excited states of  $\text{UO}_2^+$ . In addition, an analysis of the electronic structure of the ground state of  $\text{TiO}^+$  indicated the unexpected result that this system is a weak LWIR radiator. Finally, a data base for  $\text{U}^0$ ,  $\text{U}^{+1}$  and  $\text{U}^{+2}$  has been collected for examining the role of dielectronic recombination as a charge neutralization mechanism in the uranium/oxygen system (Reference 3). A brief summary of the results of our  $\text{UO}^+$  calculations performed to date follows.

Detailed searches of several symmetries of  $\text{UO}^+$  were carried out to determine the ground molecular state of this system. Our calculations indicate that the lowest symmetry of  $\text{UO}^+$  is derived from the  $(\Lambda, S)$  coupled  $^4\text{I}$  state. A vibrational analysis of the  $\Omega = 9/2$  ground state of  $\text{UO}^+$  was carried out using a Hulbert-Hirschfelder (Reference 4) fit to our calculated potential curves. The spin-orbit splittings were derived from atomic parameters for the  $\text{U}^{+3}$  ion. This fit yields an equilibrium internuclear distance of 1.84 Å and a fundamental vibrational constant of 890  $\text{cm}^{-1}$ . These data are compared with other calculated estimates, since there are no experimental data available. The agreement between our work and that of Krauss and Stevens (Reference 5) is less satisfactory than in the case of

$\text{UO}$ , but still well within the uncertainty of the several calculations.

A perturbative treatment for calculating the density of states in uranium molecules is available through the use of ligand field theory. Recent studies by Dulick (Reference 6) predict that the ground state of  $\text{UO}^+$  has  $\Omega = 9/2$ , in contrast to the effective core hamiltonian calculations of Krauss and Stevens (Reference 5) and our relativistic density functional calculations, both of which predict that the ground state has  $\Omega = 9/2$ . Again, the neglect of important molecular effects in the ligand field model apparently results in a bias toward lower  $\Omega$  values.

An analysis of the emission characteristics for the ground state of  $\text{UO}^+$  indicates an oscillator strength for emission ( $f_{10}$ ) of  $5.17 \times 10^{-5}$  at  $\lambda = 11.3 \mu$ . A complete analysis of our calculated LWIR emission for  $\text{UO}^+$  was given in DNA TR-82-159. Our calculated LWIR emission for  $\text{UO}^+$  is typical of that for a highly ionic metal oxide. We predict strong emission from the fundamentals of  $\text{UO}^+$  in the wavelength region 11 – 14  $\mu$ . Since this system exhibits weak anharmonicity, we find the overtones down in intensity by several orders of magnitude. However, the first excited state of  $\text{UO}^+$  ( $^4\text{H}$ ) lies at  $\sim 1200 \text{ cm}^{-1}$  in our calculations with a predicted electronic oscillator strength of  $\sim 1 \times 10^{-5}$  for the  $^4\text{I} - ^4\text{H}$  transition. The electronic and vibrational manifolds for  $\text{UO}^+$  are thus highly overlapped above the second vibrational level of the ground  $^4\text{I}_{9,2}$  state.

A summary of the electronic states of  $\text{UO}^+$  that have been studied, both at NBS (Krauss and Stevens) and at UTRC, is shown in Fig. 1. We find (to date) nine electronic states lying in the region .4-.8 $\mu$  that are strongly connected to either the ground  $^4\text{I}$  manifold or to the low-lying  $^4\text{I}$  manifold of  $\text{UO}^+$ . The calculated  $f$ -numbers for the bands  $1^4\text{I} \rightarrow 1^4\text{K}$ ,  $1^4\text{I} \rightarrow 3^4\text{H}$ ,  $1^4\text{I} \rightarrow 2^4\text{H}$  and  $1^4\text{I} \rightarrow 1^4\text{H}$  are given in Tables 1, 2, 3, and 4 respectively. We find a considerable shift in  $R_e$  for the  $3^4\text{H}$  state which offers a route for solar excitation followed by IR radiation. We also show in Table 4 the IR absorption corresponding to the  $1^4\text{I} \rightarrow 1^4\text{H}$  transition. Owing to the vertical nature of the potential curves, this behaves similar to a weak vibrational transition.

The photoabsorption strengths for the  $1^4\text{I} \rightarrow 2^4\text{I}$ ,  $1^4\text{I} \rightarrow 1^6\text{H}$ , and  $1^4\text{I} \rightarrow 3^4\text{I}$  transitions are presented in Tables 5 - 7, respectively. We find that the  $1^4\text{I} \rightarrow 2^4\text{I}$  oscillator strengths are large but that most of the absorbed energy will be reradiated in the visible since the transition is nearly vertical.

In contrast, the  $1^4\text{I} \rightarrow 1^6\text{H}$  transition (Table 6) is an important route for conversion of solar to IR photons, since the oscillator strength is large and the  $R_e$  of the excited state is shifted. This transition is not as strong as the  $1^4\text{I} \rightarrow 3^4\text{H}$  transition reported previously, but is a contributing factor in the total photoabsorption profile.

The  $1^4\text{I} \rightarrow 3^4\text{I}$  transition, shown in Table 7, reflects the large shift in  $R_e$  for the

excited state, but the transition moment is weak since this is an  $f \rightarrow s$  excitation on uranium.

In both the UTRC and NBS studies, a very low-lying  $^4\text{H}$  excited state is found at  $T_e \sim 1200 \text{ cm}^{-1}$ . Since this state may be thermally populated at short time conditions, the oscillator strengths coupling this  $1^4\text{H}$  state to the known six low-lying excited states of  $\text{UO}^+$  have been examined.

The calculated oscillator strengths are given in Tables 8 - 13, respectively, for the transitions:  $1^4\text{H} \rightarrow 2^4\text{I}$ ,  $1^4\text{H} \rightarrow 2^4\text{H}$ ,  $1^4\text{H} \rightarrow 1^4\text{K}$ ,  $1^4\text{H} \rightarrow 1^6\text{H}$ ,  $1^4\text{H} \rightarrow 3^4\text{H}$ , and  $1^4\text{H} \rightarrow 3^4\text{I}$ . The transitions to the  $1^4\text{K}$ ,  $1^6\text{H}$  and  $3^4\text{I}$ , show strong oscillator strengths owing to the shifted  $R_e$  for the excited states. The overall pattern of solar pumping from the  $1^4\text{H}$  state is thus very similar to that from the ground  $1^4\text{I}$  state.

Since the density of electronic states of  $\text{UO}^+$  is large above  $\sim 2.0 \text{ eV}$ , we predict that strong solar pumping, followed by both LWIR and visible radiation should occur for this system. This conclusion is similar to that reached by Krauss and Stevens (Reference 5) based on their MCSCF analysis of the  $\text{UO}^+$  system. Since several excited electronic states of  $\text{UO}^+$  lying in the region of strong solar flux (.4 - .8  $\mu$ ), exhibit shifted equilibrium internuclear separation from that of the ground  $^4\text{I}$  state, we predict efficient conversion of solar photons to IR photons for this system.

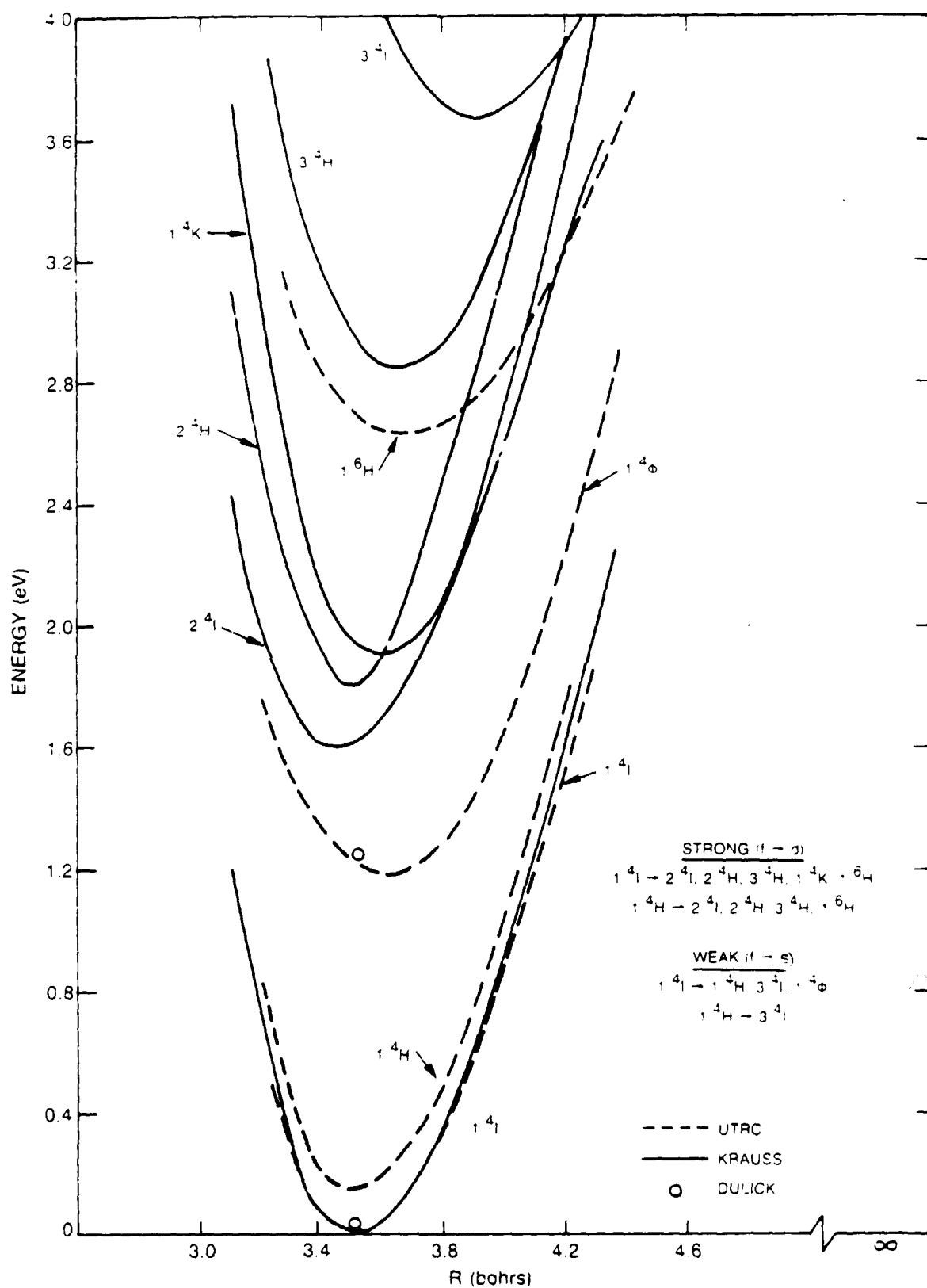


Figure 1. Potential energy curves for  $UO^+$ .

Table 1. Calculated oscillator strengths  $f_{\alpha\beta}$  for the  $1^1J - 1^1K$  transition of  $UD^+$ .

$v/v''$	0	1	2	3	4	5	6	7	8
0	*2.20-03 **0.654	1.36-03 0.694	3.99-04 0.739	6.94-05 0.790	5.21-06 0.849	6.11-08 0.916	8.29-13 0.994	5.34-10 1.086	2.10-09 1.195
1	1.54-03 0.622	3.49-04 0.658	1.33-03 0.698	6.50-04 0.744	1.48-04 0.795	1.41-05 0.854	6.94-08 0.921	3.28-08 1.00	9.54-10 1.092
2	4.54-04 0.592	1.35-03 0.625	3.66-07 0.661	1.09-03 0.701	8.69-04 0.747	2.29-04 0.798	2.30-05 0.857	3.84-08 0.924	1.47-07 1.003
3	8.93-05 0.563	8.13-04 0.593	8.13-04 0.625	1.44-04 0.661	7.52-04 0.702	1.04-03 0.747	3.25-04 0.798	3.45-05 0.856	7.60-08 0.923
4	1.95-05 0.537	2.86-04 0.564	9.24-04 0.593	3.20-04 0.625	3.85-04 0.661	4.26-04 0.701	1.15-03 0.746	4.45-04 0.797	5.51-07 0.854
5	6.61-06 0.513	8.96-05 0.538	4.88-04 0.564	7.89-04 0.593	5.30-05 0.626	5.51-04 0.661	1.68-04 0.701	1.16-03 0.746	5.96-04 0.796
6	2.97-06 0.492	3.14-05 0.514	2.03-04 0.539	6.23-04 0.565	5.36-04 0.595	3.72-06 0.627	6.04-04 0.62	2.06-05 0.762	1.04-03 0.746
7	1.20-06 0.473	1.27-05 0.494	8.26-05 0.516	3.38-04 0.540	6.66-04 0.567	2.88-04 0.596	7.97-05 0.628	5.56-04 0.664	1.20-05 0.703
8	3.07-07 0.455	4.98-06 0.475	3.38-05 0.495	1.58-04 0.518	4.61-04 0.542	6.21-04 0.569	1.18-04 0.598	1.85-04 0.630	4.42-04 0.665

\* oscillator strengths

\*\* wavelength, microns

Table 2. Calculated oscillator strengths  $f_{(v,v')}$  for the  $1^4I - 3^4H$  transition of  $UO^{+}$ .

$v/v'$	0	1	2	3	4	5	6	7	8
0	*5.61-03 **0.438	8.53-03 0.456	6.05-03 0.475	2.78-03 0.495	9.76-04 0.518	2.77-04 0.542	5.99-05 0.568	8.13-06 0.598	3.47-07 0.629
1	7.97-03 0.425	1.74-03 0.442	9.45-04 0.460	4.85-03 0.479	4.81-03 0.500	2.57-03 0.523	9.12-04 0.547	2.08-04 0.574	2.42-05 0.603
2	6.70-03 0.412	6.20-04 0.428	4.78-03 0.444	5.94-04 0.462	1.47-03 0.482	4.39-03 0.503	3.56-03 0.525	1.54-03 0.550	3.82-04 0.576
3	3.94-03 0.399	4.14-03 0.413	7.76-04 0.429	2.49-03 0.446	2.56-03 0.464	7.01-05 0.483	3.13-03 0.504	4.11-03 0.527	2.20-03 0.551
4	1.92-03 0.387	5.37-03 0.401	8.63-04 0.415	2.67-03 0.431	3.95-04 0.448	3.08-03 0.465	1.93-04 0.484	1.86-03 0.506	4.17-03 0.528
5	7.52-04 0.375	3.95-03 0.388	4.14-03 0.402	8.68-07 0.417	2.95-03 0.432	2.09-05 0.449	2.50-03 0.467	7.76-04 0.486	9.73-04 0.507
6	2.09-04 0.365	1.92-03 0.377	4.87-03 0.390	2.44-03 0.404	4.48-04 0.418	2.21-03 0.434	4.25-04 0.451	1.69-03 0.469	1.27-03 0.488
7	3.13-05 0.355	5.96-04 0.367	3.01-03 0.379	4.89-03 0.392	1.18-03 0.406	1.08-03 0.420	1.38-03 0.436	9.05-04 0.453	1.03-03 0.471
8	6.89-07 0.346	9.54-05 0.357	1.07-03 0.369	3.80-02 0.381	4.44-03 0.394	4.37-04 0.408	1.52-03 0.422	7.47-04 0.438	1.25-03 0.455

\* oscillator strengths  
\*\* wavelength, microns

Table 3. Calculated oscillator strengths  $f_{(v'v'')}$  for the  $1^1I - 2^4H$  transition of  $UO^{+}$ .

$v'/v''$	0	1	2	3	4	5	6	7	8
0	*4.21-03 **0.683	3.45-05 0.727	2.33-05 0.776	7.62-08 0.833	4.45-07 0.898	1.01-08 0.973	5.13-09 1.062	1.51-09 1.167	2.25-13 1.295
1	3.22-05 0.634	4.18-03 0.672	4.23-05 0.714	7.22-05 0.762	8.58-08 0.816	1.84-06 0.877	6.54-08 0.949	2.10-08 1.032	9.17-09 1.131
2	4.19-05 0.593	3.21-05 0.626	4.16-03 0.662	2.39-05 0.703	1.29-04 0.749	4.48-09 0.800	4.57-06 0.859	2.61-07 0.927	4.91-08 1.006
3	1.10-06 0.557	1.04-04 0.587	1.58-05 0.619	4.13-03 0.654	1.39-06 0.693	1.80-04 0.738	9.85-07 0.787	8.57-06 0.844	9.02-07 0.909
4	1.66-07 0.527	1.32-06 0.553	1.75-04 0.581	1.18-06 0.613	4.08-03 0.647	1.74-05 0.685	2.01-04 0.728	5.78-06 0.776	1.16-01 0.83
5	5.69-09 0.501	3.40-07 0.524	2.35-07 0.550	2.43-04 0.577	6.44-06 0.608	3.96-03 0.641	1.10-04 0.679	1.79-04 0.720	1.58-05 0.767
6	4.96-09 0.478	7.59-08 0.499	2.89-07 0.522	6.40-07 0.547	3.00-04 0.574	4.28-05 0.604	3.77-03 0.637	2.85-04 0.674	1.23-04 0.714
7	1.08-09 0.458	3.73-08 0.477	2.80-07 0.498	4.21-08 0.521	5.94-06 0.545	3.37-04 0.572	1.14-04 0.602	3.50-03 0.634	5.17-04 0.670
8	1.10-10 0.440	1.98-09 0.457	1.39-07 0.477	5.52-07 0.497	1.45-07 0.520	1.72-05 0.544	3.54-04 0.571	2.19-04 0.60	3.18-03 0.632

\* oscillator strengths  
 \*\* wavelength, microns

Table 4. Calculated oscillator strengths  $f_{\nu'\nu''}$  for the  $1^4I - 1^4H$  transition of  $UO^{2+}$ .

$\nu'/\nu''$	0	1	2	3	4	5	6	7	8
0	*2.73-06 **8.580	9.38-09 35.608	0. -	0. -	0. -	0. -	0. -	0. -	0. -
1	7.14-08 5.099	2.32-06 9.290	3.49-08 50.644	0. -	0. -	0. -	0. -	0. -	0. -
2	3.38-11 3.610	3.61-07 5.304	1.84-06 9.938	4.43-08 75.241	0. -	0. -	0. -	0. -	0. -
3	1.07-09 2.767	6.79-09 3.664	6.62-07 5.406	1.53-06 10.239	4.69-08 91.987	0. -	0. -	0. -	0. -
4	1.62-09 2.227	2.22-09 2.773	3.55-08 3.667	8.17-07 5.394	1.42-06 10.144	5.72-08 81.079	0. -	0. -	0. -
5	1.04-10 1.858	3.69-09 2.223	2.99-09 2.763	7.82-08 3.641	8.16-07 5.323	1.48-06 9.841	7.13-08 62.820	0. -	0. -
6	2.34-11 1.596	2.24-10 1.859	5.04-09 2.222	2.27-09 2.757	1.22-07 3.624	7.15-07 5.272	1.59-06 9.616	7.91-08 53.063	0. -
7	2.25-11 1.408	9.66-11 1.608	2.43-10 1.873	4.54-09 2.239	8.30-10 2.780	1.56-07 3.656	6.05-07 5.324	1.60-06 9.740	7.72-08 55.332
8	2.07-12 1.270	1.03-10 1.431	3.09-10 1.637	3.12-10 1.910	1.66-09 2.289	7.54-10 2.852	1.66-07 3.774	5.96-07 5.562	1.37-06 10.504

\* oscillator strengths  
 \*\* wavelength, microns

Table 5. Calculated oscillator strengths  $f(v', v'')$  for the  $1^1I - 2^1I$  transition of  $UO^+$ .

$v'/v''$	0	1	2	3	4	5	6	7	8
0	*3.55-03 **0.782	1.59-04 0.840	1.35-05 0.907	5.99-07 0.985	1.18-08 1.077	1.15-09 1.187	7.30-10 1.322	3.42-09 1.489	8.56-09 1.704
1	1.99-04 0.733	3.26-03 0.784	2.27-04 0.842	2.93-05 0.909	1.32-06 0.986	3.24-08 1.078	5.49-08 1.188	4.09-08 1.322	1.92-08 1.488
2	4.56-08 0.690	3.13-04 0.735	3.10-03 0.786	2.36-04 0.844	4.61-05 0.911	5.70-06 0.988	4.89-07 1.080	3.37-07 1.189	3.44-07 1.322
3	4.10-07 0.654	6.41-07 0.694	3.70-04 0.739	2.87-03 0.790	3.29-04 0.848	7.77-05 0.915	1.87-05 0.993	4.21-06 1.084	1.65-06 1.194
4	7.24-11 0.621	1.98-06 0.657	8.25-07 0.698	5.71-04 0.743	2.36-03 0.794	4.64-04 0.853	1.48-04 0.920	4.82-05 0.998	1.75-05 1.090
5	9.91-11 0.593	3.59-09 0.626	1.48-06 0.662	4.51-10 0.703	9.58-04 0.749	1.70-03 0.800	5.25-04 0.859	2.34-04 0.927	8.95-05 1.006
6	5.15-10 0.568	2.07-07 0.598	9.61-10 0.631	9.35-07 0.668	1.27-06 0.709	1.43-03 0.755	1.17-03 0.807	4.64-04 0.867	2.81-04 0.935
7	1.25-08 0.544	3.57-11 0.572	4.16-07 0.602	1.73-11 0.635	1.88-06 0.672	2.50-06 0.714	1.79-03 0.760	8.54-04 0.813	3.74-04 0.873
8	2.17-10 0.522	4.69-09 0.547	1.34-08 0.575	2.09-07 0.605	3.71-08 0.639	6.09-06 0.676	2.47-06 0.718	2.01-03 0.765	6.72-04 0.818

\* oscillator strength  
\*\* wavelength, microns



Table 6. Calculated oscillator strengths  $f_{(v'v'')}$  for the  $1^1I - 1^6H$  transition of  $UO^+$ .

$v'/v''$	0	1	2	3	4	5	6	7	8
0	*1.35-03 **0.480	1.66-03 0.501	1.22-03 0.524	6.43-04 0.550	2.75-04 0.577	1.05-04 0.607	3.67-05 0.641	1.09-05 0.678	2.42-06 0.719
1	2.01-03 0.468	2.56-04 0.488	1.18-04 0.509	7.02-04 0.533	8.82-04 0.559	6.45-04 0.587	3.46-04 0.619	1.49-04 0.653	5.17-05 0.691
2	1.66-03 0.456	3.81-04 0.475	8.11-04 0.495	1.72-04 0.518	6.50-05 0.542	4.66-04 0.569	6.32-04 0.598	4.91-04 0.630	2.77-04 0.666
3	6.98-04 0.445	1.50-03 0.463	2.33-05 0.482	4.04-04 0.504	5.10-04 0.527	5.34-05 0.552	1.06-04 0.579	4.39-04 0.609	5.46-04 0.642
4	1.64-04 0.434	1.40-03 0.451	7.36-04 0.470	3.70-04 0.490	3.51-05 0.512	4.75-04 0.535	2.84-04 0.561	7.65-07 0.589	1.89-04 0.620
5	1.17-05 0.423	5.30-04 0.440	1.61-03 0.458	1.49-04 0.477	5.25-04 0.497	3.81-05 0.519	2.47-04 0.544	4.15-04 0.570	8.03-05 0.599
6	2.08-07 0.413	7.46-05 0.429	9.69-04 0.446	1.34-03 0.464	1.96-06 0.483	3.93-04 0.504	2.10-04 0.527	5.59-05 0.551	3.80-04 0.578
7	1.00-06 0.403	4.21-07 0.418	2.27-04 0.434	1.33-03 0.451	8.17-04 0.470	1.28-04 0.489	1.70-04 0.511	3.53-04 0.534	7.63-07 0.559
8	2.51-07 0.394	2.70-06 0.408	1.16-05 0.423	4.77-04 0.440	1.45-03 0.457	3.19-04 0.476	2.87-04 0.496	1.93-05 0.518	3.64-04 0.542

\* oscillator strength  
\*\* wavelength, microns

Table 7. Calculated oscillator strengths  $f_{(v'v'')}$  for the  $1^1J - 3^1J$  transition of  $UO^+$ .

$v'/v''$	0	1	2	3	4	5	6	7	8
0	•2.10-07 ••0.340	1.98-06 0.351	8.93-06 0.362	2.55-05 0.374	5.23-05 0.386	8.20-05 0.400	1.03-04 0.414	1.05-04 0.429	8.91-05 0.445
1	1.31-06 0.333	9.68-06 0.343	3.23-05 0.354	6.31-05 0.365	7.81-05 0.377	6.00-05 0.390	2.33-05 0.403	7.51-07 0.417	9.63-06 0.433
2	4.73-06 0.327	2.73-05 0.336	6.64-05 0.347	8.33-05 0.357	4.96-05 0.368	5.79-06 0.379	7.90-06 0.390	4.07-05 0.401	4.94-05 0.412
3	1.20-05 0.320	5.06-05 0.329	7.98-05 0.339	4.75-05 0.349	2.00-06 0.360	2.00-05 0.372	5.21-05 0.384	2.90-05 0.397	1.93-07 0.410
4	2.35-05 0.313	6.83-05 0.322	6.00-05 0.331	6.74-06 0.341	1.56-05 0.351	4.96-05 0.362	2.01-05 0.374	1.92-06 0.386	3.42-05 0.399
5	3.39-05 0.307	6.61-05 0.315	2.66-05 0.324	1.79-06 0.334	3.61-05 0.344	2.37-05 0.354	4.97-07 0.365	2.81-05 0.377	2.31-05 0.389
6	4.94-05 0.302	6.21-05 0.310	6.96-06 0.319	1.65-05 0.328	3.48-05 0.337	2.08-06 0.347	1.84-05 0.358	2.75-05 0.369	5.25-07 0.381
7	6.74-05 0.297	4.79-05 0.305	5.87-08 0.313	3.17-05 0.322	1.54-05 0.331	4.99-06 0.341	2.98-05 0.351	4.82-06 0.362	1.19-05 0.373
8	8.20-05 0.292	2.80-05 0.300	7.80-06 0.308	3.21-05 0.317	1.12-06 0.326	1.99-05 0.335	1.61-05 0.345	2.18-06 0.355	2.40-05 0.366

• oscillator strength  
•• wavelength, microns

Table 8. Calculated oscillator strengths  $f_{(v,v')}$  for the  $1^1B_1 - 2^1A_1$  transition of  $UO^+$ .

$v'/v''$	0	1	2	3	4	5	6	7	8
0	*2.83-03 **0.860	2.79-04 0.923	3.33-05 0.998	7.19-06 1.090	1.86-06 1.205	2.12-07 1.356	3.79-10 1.532	2.18-09 1.758	3.43-10 2.034
1	3.65-04 0.802	2.03-03 0.856	6.19-04 0.920	1.05-04 0.997	1.92-05 1.093	3.97-06 1.211	6.37-07 1.355	6.24-08 1.529	1.55-09 1.734
2	9.71-06 0.751	8.63-04 0.798	1.29-03 0.854	7.74-04 0.920	1.72-04 1.000	3.65-05 1.099	9.06-06 1.216	1.58-06 1.355	3.06-07 1.513
3	1.52-06 0.708	5.69-05 0.750	1.14-03 0.798	7.28-04 0.856	8.46-04 0.925	2.65-04 1.008	6.42-05 1.107	2.10-05 1.220	5.21-06 1.347
4	1.98-07 0.670	3.95-06 0.707	1.49-04 0.750	1.32-03 0.801	3.16-04 0.862	7.48-04 0.933	3.76-04 1.017	1.10-04 1.111	4.40-05 1.216
5	4.99-08 0.637	8.74-07 0.671	1.23-05 0.710	2.82-04 0.755	1.44-03 0.808	9.38-05 0.871	5.08-04 0.943	4.35-04 1.024	1.65-04 1.112
6	5.90-09 0.608	3.68-10 0.639	1.14-06 0.674	1.73-05 0.714	4.04-04 0.762	1.56-03 0.817	2.14-05 0.881	2.75-04 0.951	4.01-04 1.026
7	2.44-08 0.581	7.55-08 0.609	1.60-07 0.641	6.25-09 0.677	8.93-06 0.720	4.64-04 0.770	1.67-03 0.826	4.19-06 0.887	1.49-04 0.952
8	1.70-09 0.556	5.13-09 0.582	6.62-07 0.610	1.91-06 0.644	4.04-06 0.682	5.74-07 0.726	4.91-04 0.776	1.70-03 0.830	1.87-06 0.887

\* oscillator strength

\*\* wavelength, microns

Table 9. Calculated oscillator strengths  $f_{(v'v'')}$  for the  $1^1H - 2^4H$  transition of  $UO^{+}$ .

$v/v''$	0	1	2	3	4	5	6	7	8
0	*3.63-03 **0.742	1.14-05 0.788	3.41-05 0.842	1.94-06 0.907	6.01-07 0.985	1.25-07 1.080	7.50-09 1.193	7.43-09 1.326	1.94-11 1.477
1	4.34-06 0.685	3.48-03 0.724	2.05-04 0.769	4.60-05 0.823	9.64-06 0.887	1.11-06 0.963	5.33-07 1.052	8.61-09 1.154	3.44-08 1.267
2	5.54-05 0.637	1.22-04 0.672	3.02-03 0.709	5.66-04 0.755	3.13-05 0.808	2.13-05 0.871	1.17-06 0.944	1.38-06 1.025	5.49-11 1.113
3	2.90-06 0.597	1.63-04 0.626	2.84-04 0.660	2.46-03 0.699	9.16-04 0.744	1.02-05 0.797	3.37-05 0.858	4.82-07 0.924	2.86-06 0.995
4	2.99-07 0.562	2.36-05 0.588	2.87-04 0.618	3.95-04 0.652	2.01-03 0.691	1.16-03 0.737	6.84-10 0.788	4.36-05 0.843	1.87-07 0.902
5	9.46-08 0.532	2.45-06 0.556	6.24-05 0.582	3.77-04 0.612	4.64-04 0.646	1.70-03 0.686	1.28-03 0.730	1.73-05 0.778	4.31-05 0.827
6	1.15-09 0.506	3.11-07 0.527	5.36-06 0.551	9.67-05 0.578	4.25-04 0.609	5.27-04 0.644	1.45-03 0.682	1.35-03 0.724	8.71-05 0.766
7	2.24-09 0.484	2.68-09 0.503	1.32-07 0.524	5.07-06 0.549	1.13-04 0.576	4.56-04 0.607	6.08-04 0.642	1.14-03 0.678	1.43-03 0.716
8	7.74-10 0.463	4.33-08 0.482	1.58-07 0.501	1.36-07 0.523	2.32-06 0.548	1.18-04 0.576	5.05-04 0.607	7.02-04 0.639	6.85-04 0.673

\* oscillator strength  
\*\* wavelength, microns

Table 10. Calculated oscillator strengths  $f(v'v'')$  for the  $^{14}\text{H} - ^{14}\text{K}$  transition of  $\text{UO}^+$ .

$v'/v''$	0	1	2	3	4	5	6	7	8
0	2.49-03 * 0.708 **	1.18-03 0.750	1.07-04 0.799	8.12-07 0.857	4.40-08 0.926	5.64-08 1.010	5.93-08 1.108	2.66-10 1.222	1.93-09 1.349
1	1.13-03 0.671	1.15-03 0.708	1.36-03 0.751	1.74-04 0.802	5.49-06 0.863	1.54-07 0.935	2.51-07 1.019	1.59-07 1.114	4.97-10 1.219
2	2.85-04 0.636	1.06-03 0.670	6.81-04 0.708	1.48-03 0.753	2.78-04 0.806	1.91-05 0.869	1.98-06 0.941	7.29-07 1.021	1.08-07 1.108
3	4.95-05 0.603	3.83-04 0.633	1.06-03 0.667	2.92-04 0.707	1.50-03 0.754	4.52-04 0.808	5.35-05 0.870	6.53-06 0.939	7.17-07 1.012
4	7.41-06 0.573	1.06-04 0.600	4.75-04 0.630	1.02-03 0.666	3.96-05 0.707	1.33-03 0.755	6.78-04 0.809	1.13-04 0.867	9.25-06 0.930
5	1.58-06 0.546	2.24-05 0.571	1.73-04 0.598	5.77-04 0.630	8.41-04 0.667	2.42-05 0.709	1.02-03 0.756	9.22-04 0.807	1.72-04 0.861
6	5.65-07 0.522	4.89-06 0.545	4.91-05 0.570	2.57-04 0.598	6.90-04 0.632	5.18-04 0.669	1.91-04 0.711	7.39-04 0.756	1.12-03 0.803
7	1.97-07 0.501	1.50-06 0.521	1.15-05 0.544	9.73-05 0.570	3.63-04 0.600	7.57-04 0.634	2.00-04 0.672	3.17-04 0.712	5.95-04 0.754
8	3.66-08 0.481	4.64-07 0.500	3.24-06 0.521	2.62-05 0.545	1.68-04 0.573	4.80-04 0.603	7.02-04 0.637	3.63-05 0.673	3.21-04 0.710

\* oscillator strength

\*\* wavelength, microns

Table 11. Calculated oscillator strengths  $f_{(v',v'')}$  for the  $1^4H - 1^6H$  transition of  $UO^+$ .

$v'/v''$	0	1	2	3	4	5	6	7	8
0	*1.76-03 **0.508	2.05-03 0.530	9.07-04 0.554	2.58-04 0.581	8.70-05 0.612	4.05-05 0.647	1.99-05 0.686	7.62-06 0.728	1.40-06 0.772
1	1.96-03 0.494	1.38-05 0.515	7.37-04 0.537	1.03-03 0.563	6.01-04 0.592	3.25-04 0.625	1.91-04 0.661	1.04-04 0.700	3.47-05 0.740
2	1.28-03 0.481	9.93-04 0.500	5.28-04 0.521	2.05-05 0.545	4.44-04 0.573	5.41-04 0.604	4.74-04 0.638	3.78-04 0.674	2.13-04 0.711
3	4.53-04 0.469	1.43-03 0.487	2.79-04 0.507	7.35-04 0.530	1.61-04 0.556	4.62-05 0.585	3.05-04 0.616	5.30-04 0.650	5.55-04 0.684
4	8.78-05 0.457	7.57-04 0.474	1.55-03 0.493	1.40-06 0.515	4.47-04 0.539	4.53-04 0.566	2.94-05 0.596	1.05-04 0.627	4.66-04 0.659
5	2.50-06 0.445	1.64-04 0.462	1.08-03 0.480	1.30-03 0.500	1.29-04 0.523	9.53-05 0.548	4.58-04 0.576	1.45-04 0.605	3.19-05 0.635
6	2.14-06 0.434	5.79-06 0.449	2.52-04 0.466	1.49-03 0.486	7.34-04 0.507	3.35-04 0.531	2.90-06 0.557	2.97-04 0.585	2.15-04 0.612
7	2.44-06 0.423	4.71-06 0.438	1.08-05 0.454	4.30-04 0.472	1.76-03 0.492	1.95-04 0.515	3.43-04 0.539	8.36-05 0.565	1.76-04 0.591
8	5.53-07 0.413	6.57-06 0.427	5.82-06 0.442	2.49-05 0.459	7.82-04 0.479	1.58-03 0.500	5.26-07 0.523	1.99-04 0.547	1.52-04 0.571

\* oscillator strength  
 \*\* wavelength, microns

Table 12. - Calculated oscillator strengths  $f_{(v'v'')}$  for the  $1^4H - 3^4H$  transition of  $UO^+$ .

$v'/v''$	0	1	2	3	4	5	6	7	8
0	*7.31-03 **0.462	1.02-02 0.480	4.04-03 0.499	8.66-04 0.521	2.13-04 0.546	7.59-05 0.574	2.62-05 0.604	5.68-06 0.637	1.27-07 0.669
1	7.62-03 0.448	1.48-04 0.464	5.03-03 0.482	5.90-03 0.503	2.45-03 0.526	8.82-04 0.552	3.55-04 0.580	1.11-04 0.610	1.06-05 0.640
2	5.20-03 0.433	2.67-03 0.448	3.10-03 0.465	7.42-04 0.484	4.57-03 0.506	3.50-03 0.530	1.74-03 0.556	7.48-04 0.583	1.66-04 0.610
3	2.78-03 0.419	4.57-03 0.433	3.28-04 0.449	4.62-03 0.466	1.28-04 0.486	2.27-03 0.508	3.87-03 0.532	2.69-03 0.557	1.06-03 0.582
4	1.27-03 0.405	3.74-03 0.419	3.48-03 0.433	1.22-04 0.450	3.61-03 0.468	1.36-03 0.489	7.00-04 0.511	3.84-03 0.533	3.40-03 0.556
5	4.39-04 0.393	2.12-03 0.405	4.20-03 0.419	2.30-03 0.434	1.07-03 0.452	1.69-03 0.471	2.18-03 0.491	1.86-04 0.512	4.06-03 0.533
6	9.12-05 0.381	7.71-04 0.393	2.79-03 0.406	4.54-03 0.420	1.17-03 0.436	2.04-03 0.454	4.20-04 0.473	2.04-03 0.493	1.29-04 0.512
7	5.36-06 0.370	1.39-04 0.382	1.07-03 0.394	3.41-03 0.407	4.63-03 0.423	3.38-04 0.439	2.36-03 0.457	3.55-05 0.475	1.62-03 0.493
8	8.92-07 0.361	3.59-06 0.371	1.75-04 0.383	1.39-03 0.395	4.05-03 0.410	4.26-03 0.425	7.88-06 0.442	2.08-03 0.459	4.45-07 0.476

\* oscillator strength  
\*\* wavelength, microns

Table 13. Calculated oscillator strengths  $f_{(v'v'')}$  for the  $1^4I_1 - 3^4I_1$  transition of  $UO^{2+}$ .

$v'/v''$	0	1	2	3	4	5	6	7	8
0	•7.55-07 ••0.354	8.06-06 0.365	2.82-05 0.376	5.43-05 0.388	7.68-05 0.402	9.61-05 0.417	1.16-04 0.432	1.31-04 0.449	1.12-04 0.465
1	3.94-06 0.346	3.15-05 0.356	7.72-05 0.367	9.30-05 0.379	6.94-05 0.392	3.34-05 0.406	5.73-06 0.421	4.19-06 0.436	5.00-05 0.452
2	1.21-05 0.340	7.14-05 0.349	1.16-04 0.359	7.13-05 0.370	1.24-05 0.383	2.24-06 0.396	2.89-05 0.411	5.38-05 0.425	3.50-05 0.440
3	2.58-05 0.332	1.02-04 0.341	8.46-05 0.351	7.55-06 0.361	1.58-05 0.373	5.36-05 0.386	4.30-05 0.400	4.73-06 0.414	1.73-05 0.427
4	4.29-05 0.325	1.03-04 0.333	2.67-05 0.342	1.21-05 0.353	6.35-05 0.364	3.91-05 0.376	6.57-07 0.389	2.18-05 0.402	3.73-05 0.415
5	5.43-05 0.318	7.51-05 0.326	8.03-07 0.335	4.38-05 0.345	4.42-05 0.356	1.27-06 0.367	1.92-05 0.380	3.09-05 0.392	1.15-06 0.404
6	7.13-05 0.313	5.27-05 0.321	5.78-06 0.329	5.50-05 0.338	1.11-05 0.349	1.19-05 0.360	3.81-05 0.372	7.68-06 0.383	1.13-05 0.396
7	8.88-05 0.307	2.73-05 0.315	2.56-05 0.323	3.75-05 0.332	9.66-07 0.342	3.80-05 0.353	1.98-05 0.364	2.55-06 0.376	2.50-05 0.387
8	1.00-04 0.303	8.07-06 0.310	4.20-05 0.318	1.19-05 0.327	1.85-05 0.336	3.43-05 0.347	5.02-07 0.358	2.06-05 0.369	1.13-05 0.380

• oscillator strength  
•• wavelength, microns



## SECTION 2

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